2-Chloronaphthalene 91-58-7 | DTXSID8023971

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 3.45

Global applicability domain: Inside

Local applicability domain index: 6.31e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

Image not found

2,6-Dichlorotoluene Measured: 3.99 Predicted: 3.58

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Benzene, 1,4-dichloro-2-methyl-

Measured: 3.97 Predicted: 3.53

Image not found

2,4-Dichlorotoluene Measured: 4.24 Predicted: 3.54

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Ethanone, 1-(4-bromophenyl)-

Measured: 2.43 Predicted: 2.48

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3'-Bromoacetophenone

Measured: 2.47 Predicted: 2.50